

Background

Ge has a nearly direct bandgap: the energy difference between the direct bandgap and the indirect bandgap is very small (~140 meV). Tensile strain and alloying are the two most common approaches to make Ge-based direct bandgap materials.

Although $Ge_{1-x}Sn_x$ becomes a direct bandgap material with $x > 8\%$, strained growth on Ge or GaAs adds undesirable compressive strain.^{1,2} Worse, the very small electron effective mass ($m_e^* \approx 0.02m_0$) loses the direct bandgap when confined in a quantum well or dot.³

Our group has previously demonstrated that $Ge_{1-y}C_y$ with $y \approx 1\%$ has a direct bandgap, and we previously grew GeC using a special precursor (4GeMe) as a C source with no defects detectable in TEM^{4,5}.

In this work, we instead grew $Ge_{1-x-y}Sn_xC_y$ using commercially available carbon tetrabromide (CB_{r4}). GeSnC adds additional control in epitaxial growth: Sn and C partially compensate local strain and distortion of the host Ge bonds. This is likely to increase both C and Sn substitutional incorporation and provides a more stable material.

We believe C-C pairs are likely defects in the carbon containing alloys, so we also used atomic hydrogen to help reduce those defects.

These results suggest two routes to direct bandgap Group IV materials for active silicon photonics such as lasers and amplifiers.

Research Problem

Group III-V semiconductors provide superior optoelectronic properties owing to their direct bandgap and this enables their versatile uses in photonic devices such as laser, amplifiers etc. However, they have a different crystal structure from Si which introduces significant challenges in integration of those devices on Si. Unlike group III-V materials, all group IV semiconductors are indirect bandgap and that's why they are poor light emitters. Therefore, the motivation of this project is to develop a direct bandgap group IV material which can be later used in Si photonics as a laser source.

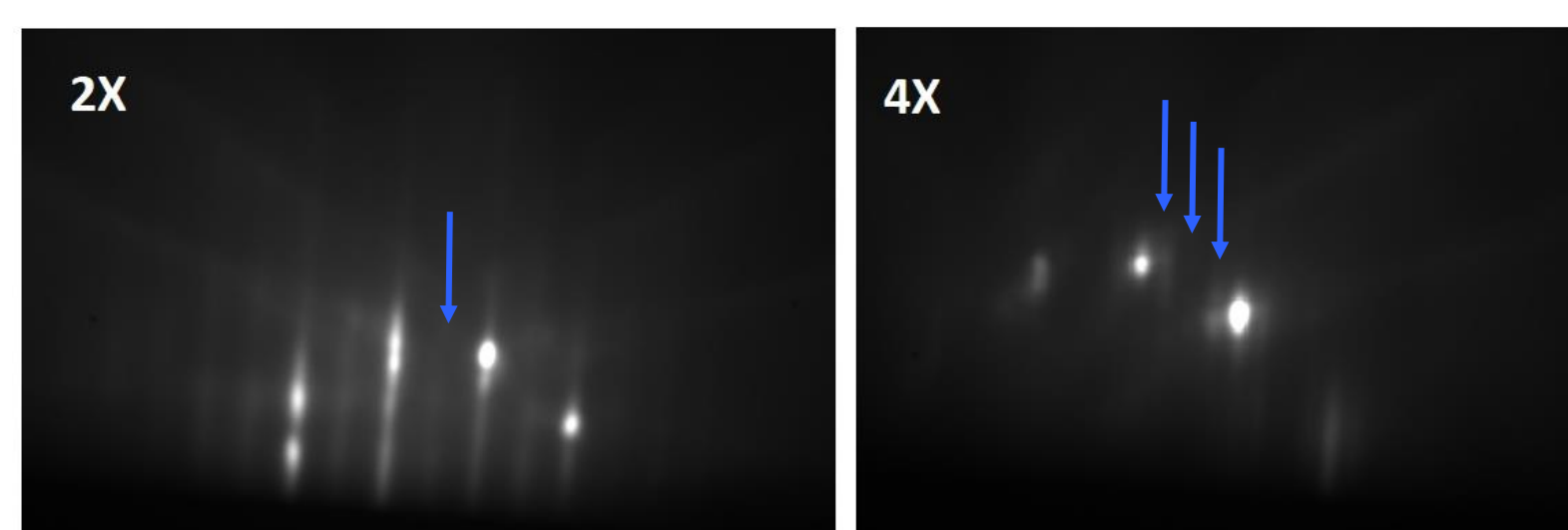
Growth Method

Growth method: Molecular Beam Epitaxy
 Solid source: Ge, Sn
 Gas source: CB_{r4} , Atomic hydrogen source
 Base pressure: 1×10^{-9} Torr
 Growth temperature: 215 °C

Beam flux and shutter were used for composition and thickness control
 Atomic hydrogen was used for oxide desorption

Ge Cap (10 nm)
GeSnC (200 nm)
Ge Buffer (150 nm)
GaAs (sub)

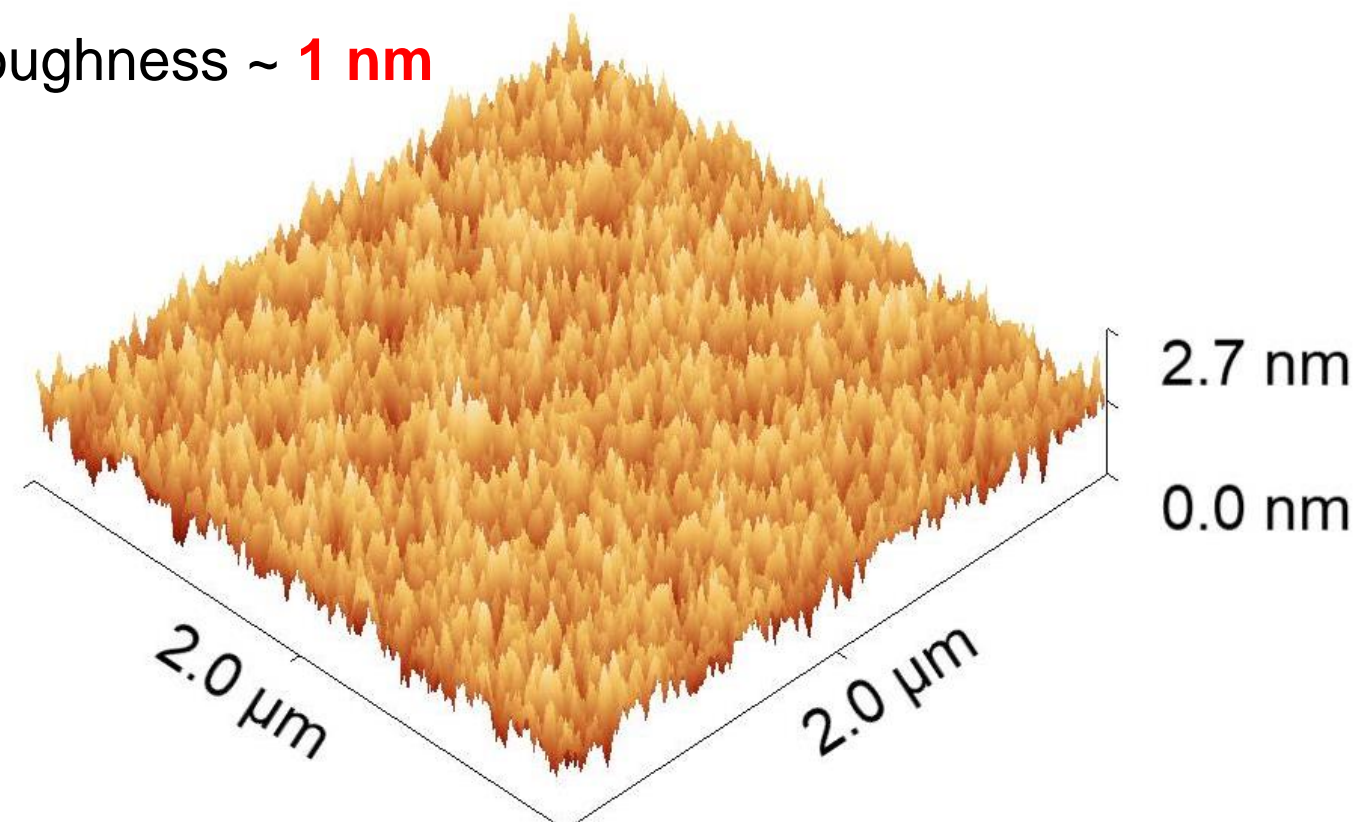
In-situ RHEED demonstrated flat **oxide free surface** reconstruction (2×4)



Native oxide desorption from GaAs substrate

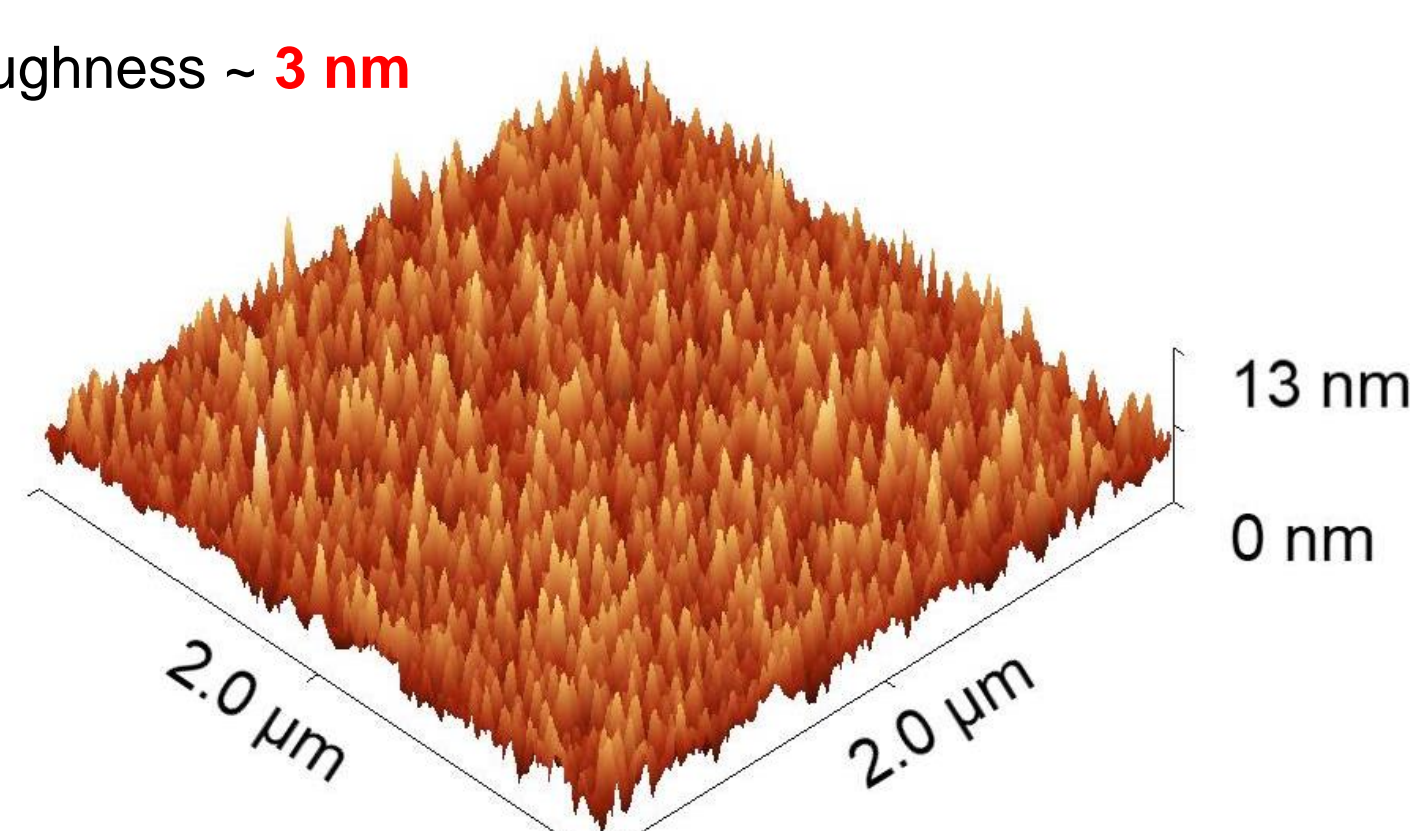
Surface Morphology: Atomic Force Microscopy

RMS Roughness ~ 1 nm



AFM image of GeSnC surface without atomic H

RMS Roughness ~ 3 nm

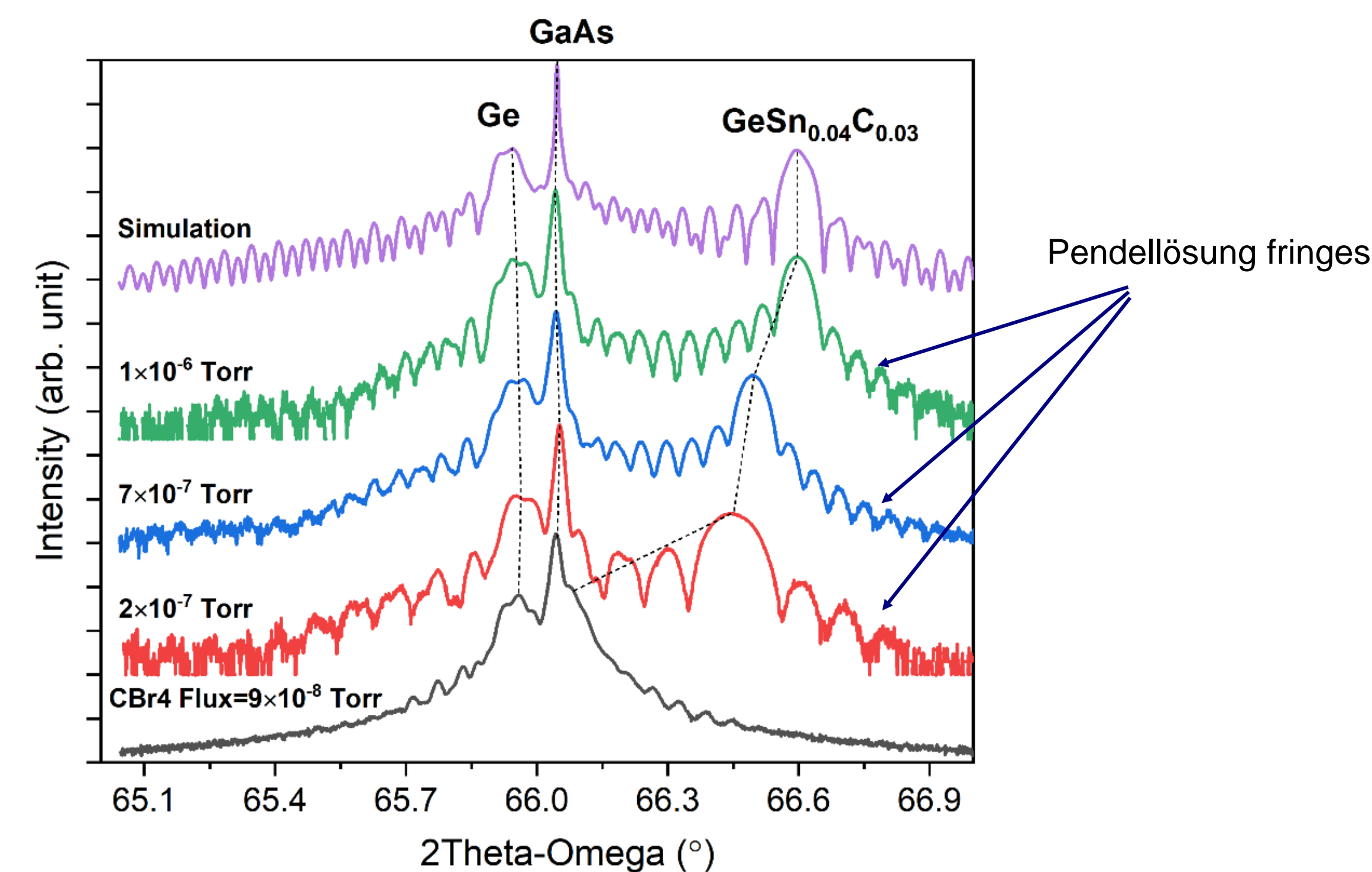


AFM image of GeSnC surface with atomic H

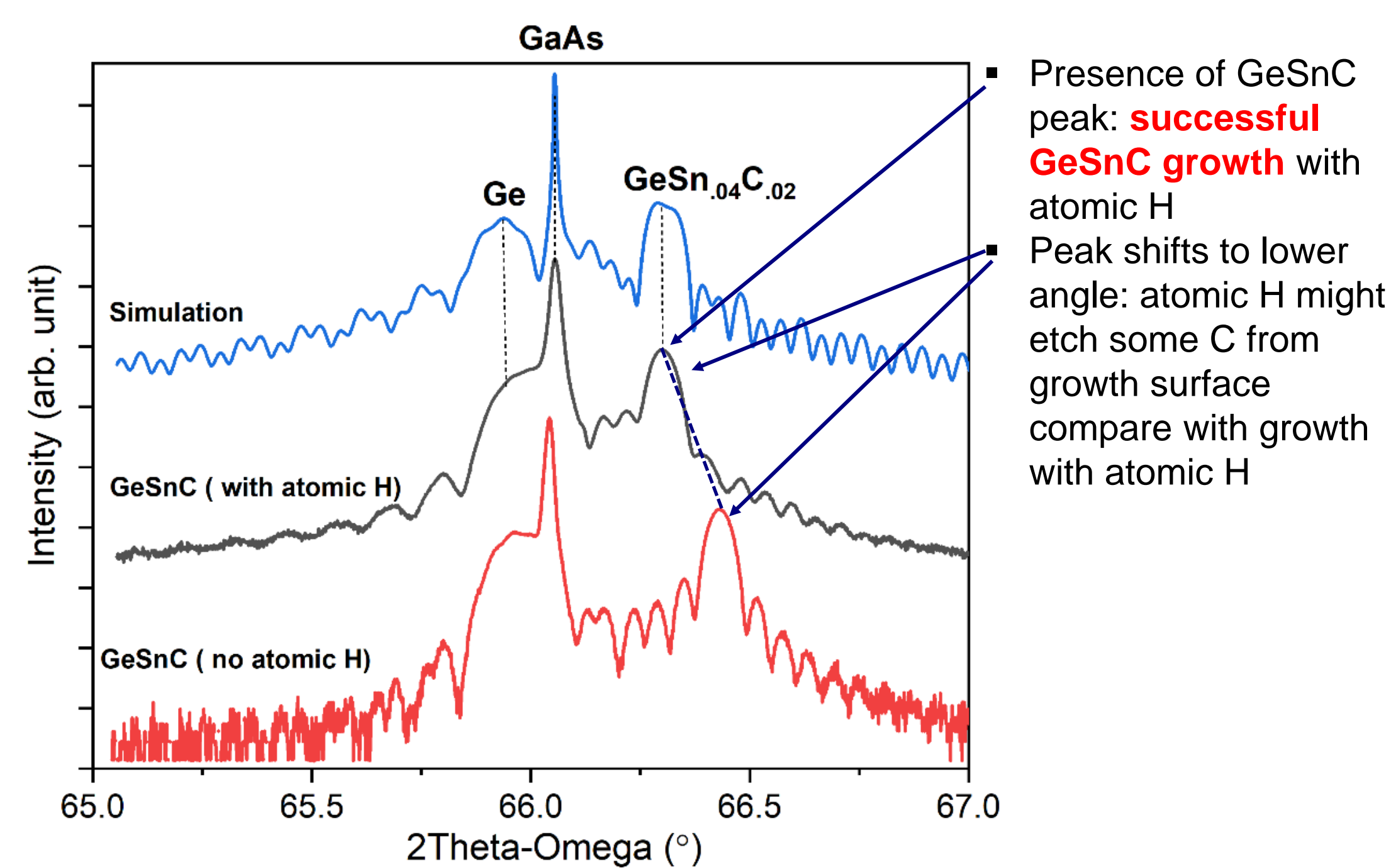
✓ **Atomically flat surface** in both approaches (with or without atomic H)

Crystal Quality: XRAY Diffraction (XRD)

- At low CB_{r4} flux the carbon incorporation is lower
- At high CB_{r4} flux, GeSnC peak **shifts** to higher angle indicating higher substitutional carbon incorporation
- Substitutional incorporation** (simulated): **Sn= 4%** and **C=3%**
- Pendellösung fringes are present in all sample indicating **flat and coherent interface**
- Line width** (FWHM) GeSnC is small (**~42 arc-sec**) indicating **good crystal quality**



XRD ω - 2θ scans about GaAs (004) Bragg reflection as a function of CB_{r4} fluxes



XRD ω - 2θ scans about GaAs (004) Bragg reflection with and without atomic H

- ✓ Possible to grow **High Crystal Quality** GeSnC epitaxial layer with or without atomic H
- ✓ Minimum substitutional content achieved: **Sn= 4%** and **C=3%**

Conclusions/Future Work

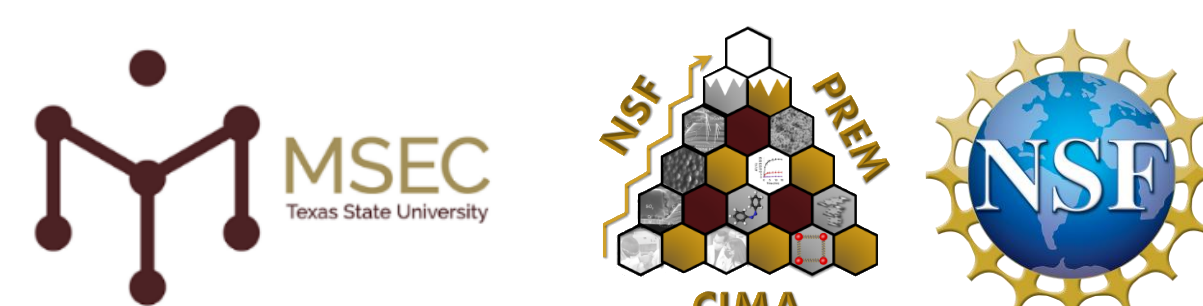
- Rutherford backscattering spectrometry (RBS): Quantifying C-C defects
- Photoluminescence (PL): Quantifying other kind of defects
- Secondary Ion Mass Spectrometry (SIMS): Quantifying total contents

References

- G. Grzybowski, et al., Next generation of $Ge_{1-y}Sn_y$ ($y = 0.01-0.09$) alloys grown on Si(100) via Ge_3H_6 and SnD_4 : Reaction kinetics and tunable emission, Applied Physics Letters, 101 (2012).
- R. Chen et al., Increased photoluminescence of strain-reduced, high-Sn composition $Ge_{1-x}Sn_x$ alloys grown by molecular beam epitaxy, Applied Physics Letters, 99 (2011) 181125.
- M.P. Polak, et al., The electronic band structure of $Ge_{1-y}Sn_y$ in the full composition range: indirect, direct, and inverted gaps regimes, band offsets, and the Burstein-Moss effect, Journal of Physics D: Applied Physics, 50 (2017).
- C.A. Stephenson, M.A. Wistey et al., Band Anticrossing in Dilute Germanium Carbides Using Hybrid Density Functionals, Journal of Electronic Materials, 45 (2015) 2121-2126.
- C.A. Stephenson, M.A. Wistey et al., Band structure of germanium carbides for direct bandgap silicon photonics, Journal of Applied Physics, 120 (2016).

Acknowledgements

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Substitutional C: Raman Spectroscopy

- Ge-Sn peak at 263 cm^{-1} is wide and hidden by shoulder of Ge-Ge peak
- Substitutional Ge-C** incorporation is verified by Raman Peak at **530 cm^{-1}**

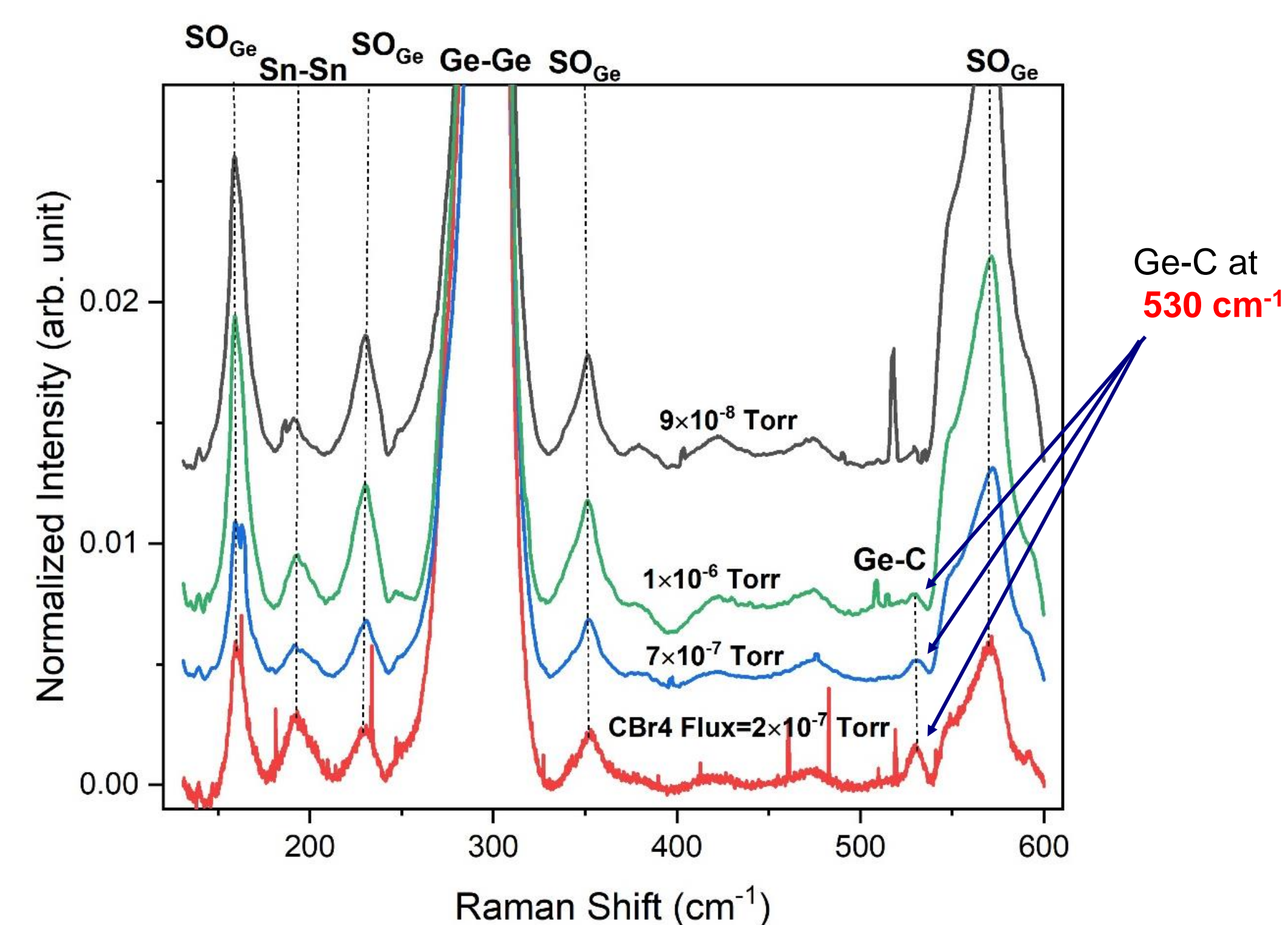
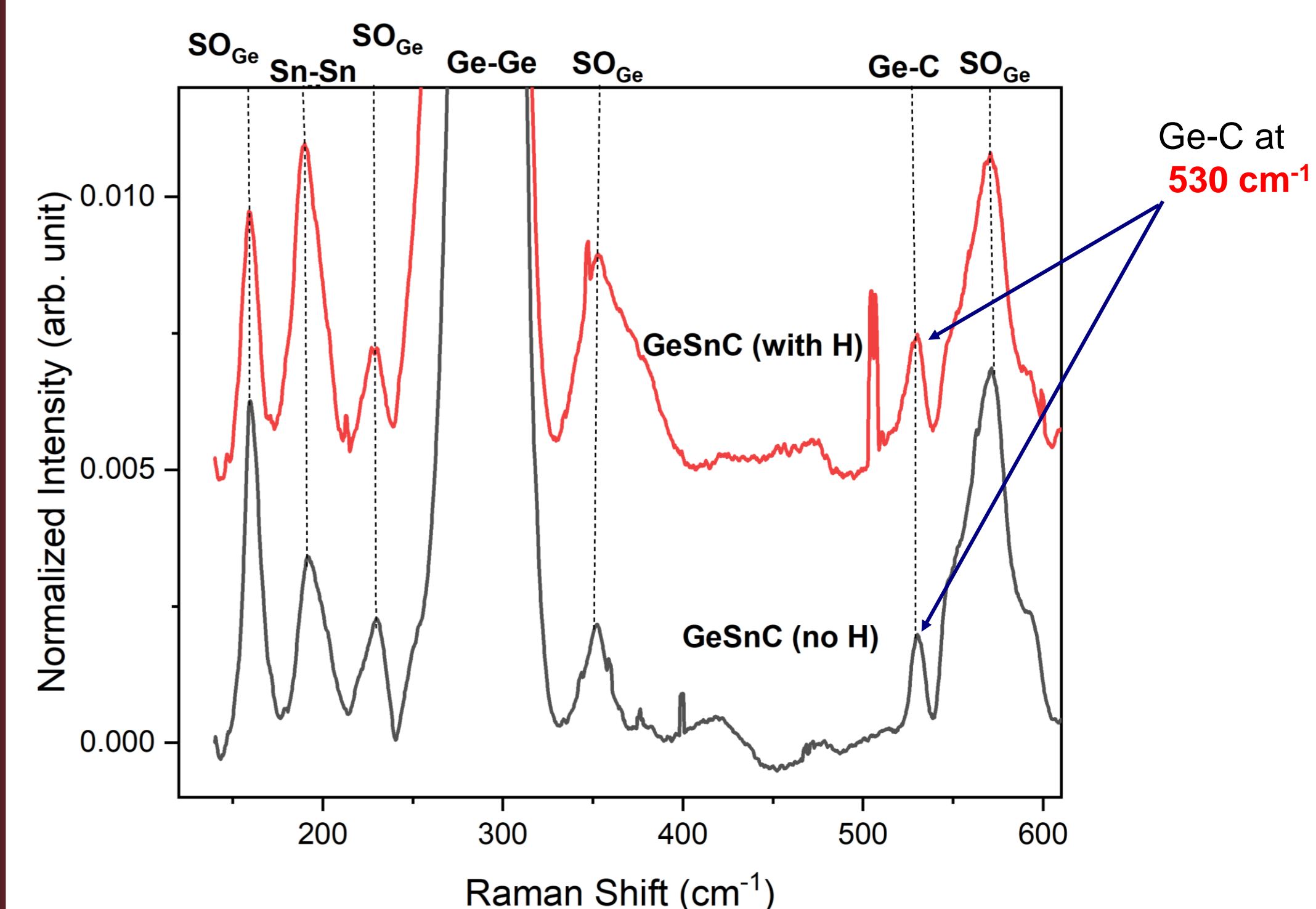


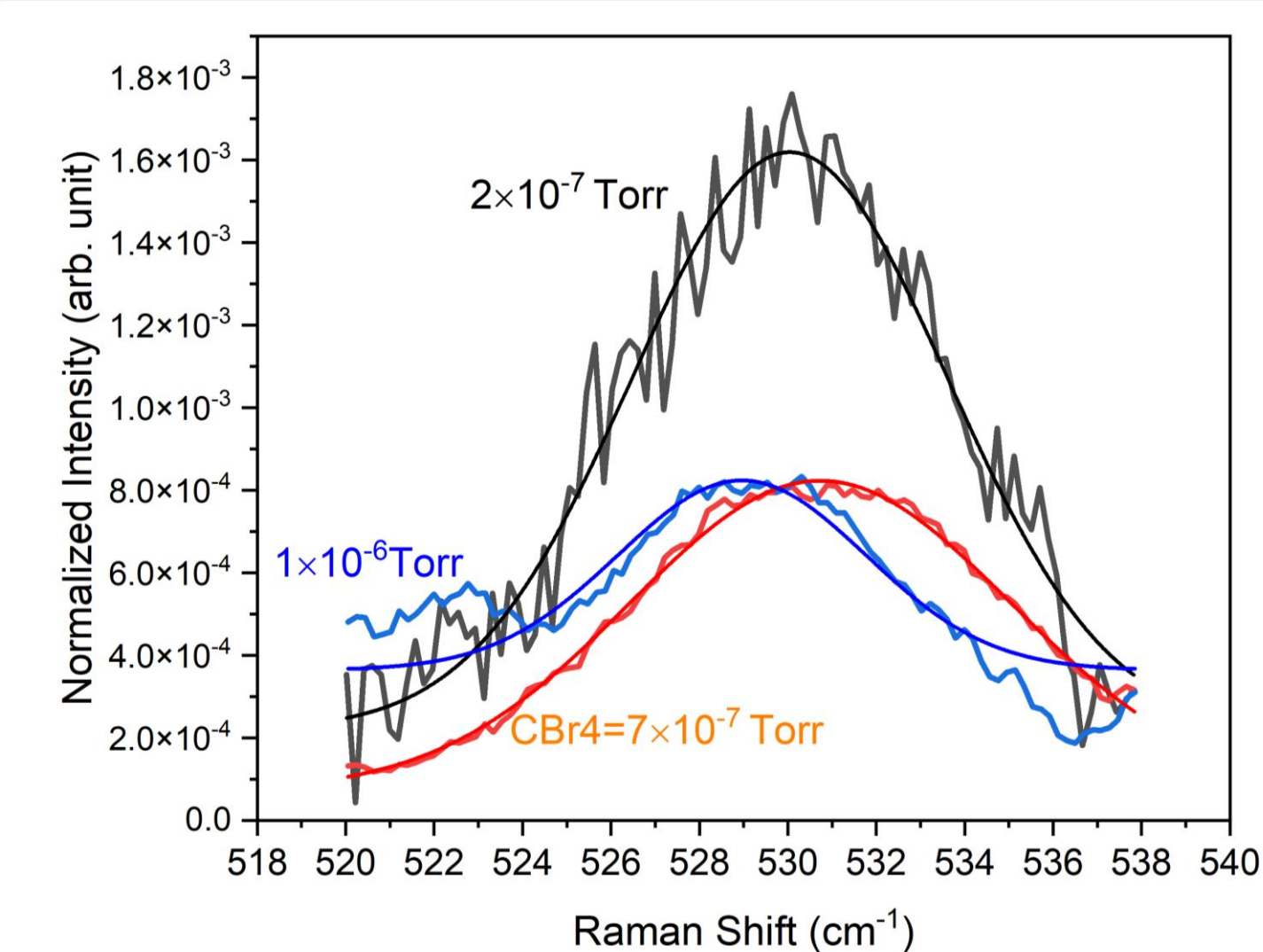
Fig. 5 Raman spectra of GeSnC as a function of CB_{r4} fluxes



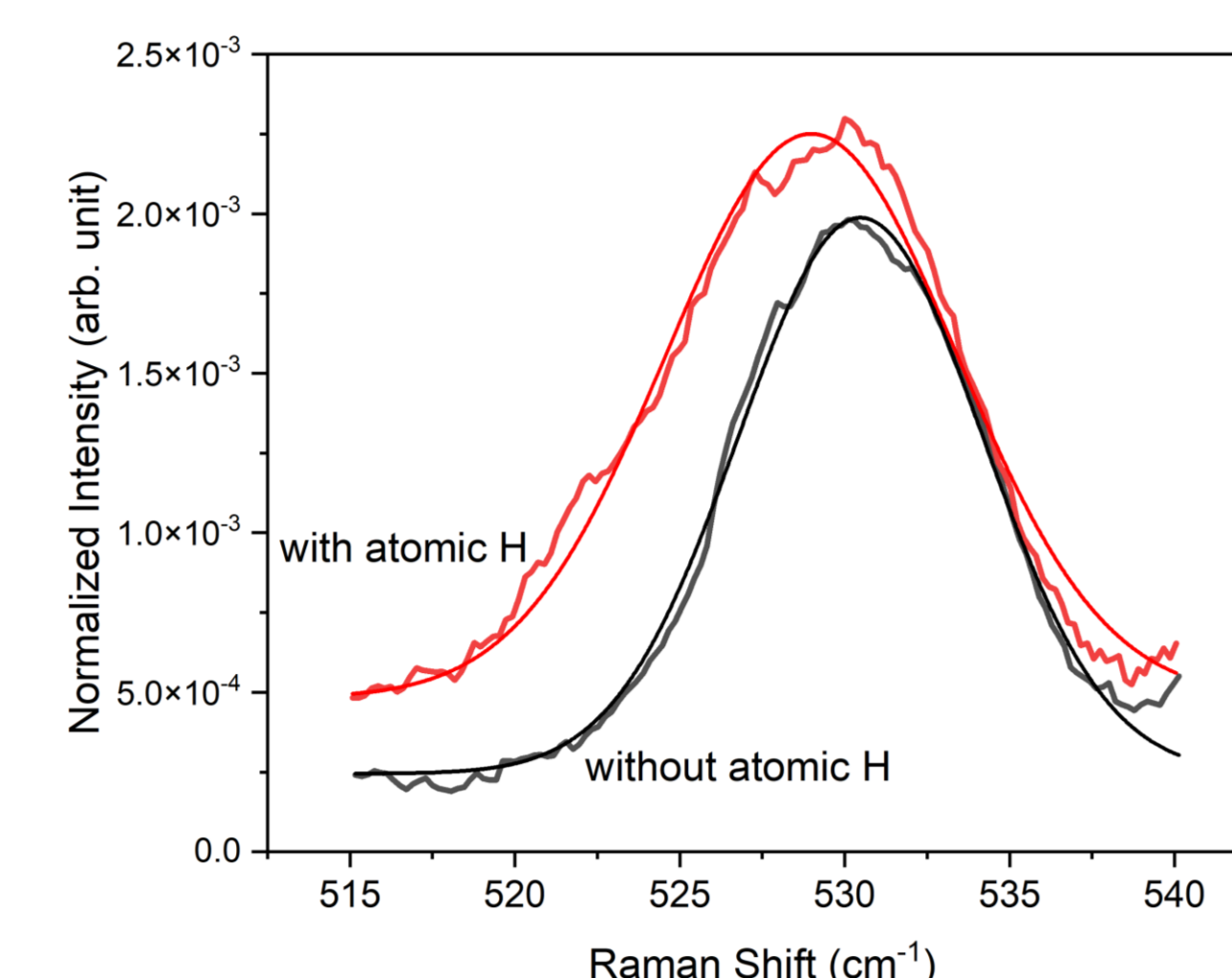
Raman spectra of GeSnC with and without atomic H

- ✓ C incorporation can be **controlled** by CB_{r4} flux
- ✓ Both approaches (with or without atomic H) can incorporate **substitutional C**

Substitutional C: Raman Spectroscopy (cont.)



Ge-C at 530 cm^{-1} of variable CB_{r4} fluxes with Gaussian peak fitting



Ge-C at 530 cm^{-1} with Gaussian peak fitting

- ✓ Ge-C peak for substitutional carbon is **well fitted** with Gaussian fitting
- ✓ Both approaches (with or without atomic H) has small FWHM (**~9 cm^{-1}**) which indicates good crystal quality